

Propanoic acid, 2-(1-oxopropoxy)-, methyl ester  
61402-72-0 | DTXSID30485366

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	1.14	0.85	1.12	0.83	1.23

## Model Results

**Predicted value:**  $4.09\text{e-}12\text{ cm}^3/\text{molecule}\cdot\text{sec}$

**Global applicability domain:** Inside

**Local applicability domain index:**  $5.92\text{e-}01$

**Confidence level:**  $7.42\text{e-}01$

## Nearest Neighbors from the Training Set

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Dimethyl glutarate

**Measured:**  $3.30\text{e-}12$

**Predicted:**  $3.76\text{e-}12$

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Dimethyl adipate

**Measured:**  $8.40\text{e-}12$

**Predicted:**  $6.84\text{e-}12$

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Dimethyl succinate

**Measured:**  $1.40\text{e-}12$

**Predicted:**  $1.93\text{e-}12$

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Ethyl 3-ethoxypropionate

**Measured:**  $2.29\text{e-}11$

**Predicted:**  $1.63\text{e-}11$

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Ethyl lactate

**Measured:**  $3.90\text{e-}12$

**Predicted:**  $4.80\text{e-}12$